Atomic-Level Characterization of Advanced Aluminum Alloys

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A research team led by an NCEM visitor from Belgrade University employed quantitative high resolution microscopy to characterize advanced aluminum alloys for use in aerospace technologies. The group analyzed and refined the crystal structure of minute inclusions only nanometers in size, and has shown how this structure leads to the shape and distribution of the strengthening phase.

Background - Aluminum-based alloys are attractive for use in automotive and aerospace applications because of their light weight and low cost. To overcome their inherent softness, the aluminum matrix is strengthened by a fine dispersion of second phase precipitates whose size, shape and distribution control the mechanical properties of the alloy. One of the most advanced aluminum alloys uses the so-called S-phase for dispersion strengthening. However, until now, the low volume fraction and small size of this phase has prevented a complete understanding of its structure, limiting the control and optimization of this class of alloy.

Accomplishment - The current study employed quantitative atomic resolution microscopy to solve the controversy over the structure of the S-phase in Al alloys containing Cu and Mg. The group was able to analyze the atomic structure of precipitates only a few nanometers in size. Using the resulting structure model it was shown that two different precipitate shapes were stable, leading to a particularly even distribution of precipitates as desired for good mechanical properties.

High resolution images such as those shown here were recorded on NCEM's atomic resolution microscopes. Segments of such micrographs of nanoscale S-phase precipitates were digitized for quantitative analysis.

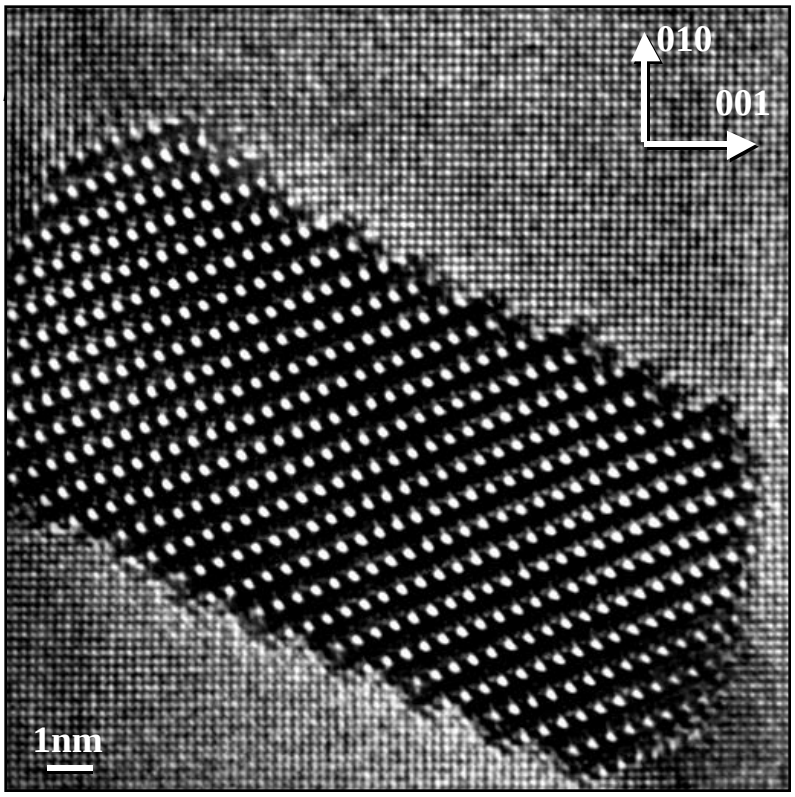
The as-recorded electron micrograph shown at the left is limited by image “noise”. Using a technique known as "crystallographic image processing" the signal to noise level was enhanced significantly by enforcing known symmetries of the structure. The resulting symmetrized image was then compared to simulated model images, employing a custom-developed optimization technique to find the best model.

The optimization process is complex because the experimental image depends upon many independent parameters such as the sample thickness, electron optical parameters and the atomic coordinates. The quality of the model can be judged by how closely the simulated image fits the experimentally observed image. This is shown visually with an inset (framed) of a simulated image from the optimized model. A quantitative measure of the fit is given by the cross correlation coefficient which is plotted as a function of the Cu/Mg exchange ratio. Compared with the previously accepted model, the new model reverses the position of the Cu and Mg atoms while making only small adjustments to the lattice parameters and the atomic positions within the unit cell (see table).

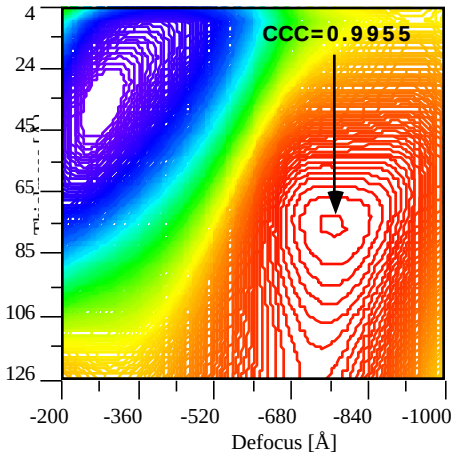
Using the new crystallographic structure, the research group was able to find an atomic correspondence between the matrix and precipitate lattices which for the first time fully explains the observed shapes and orientations of the S-phase precipitates.

This study is one of the first instances where structure refinement by electron microscopy has been applied to precipitates as small as a few nanometers. It is expected that the techniques developed here will become important

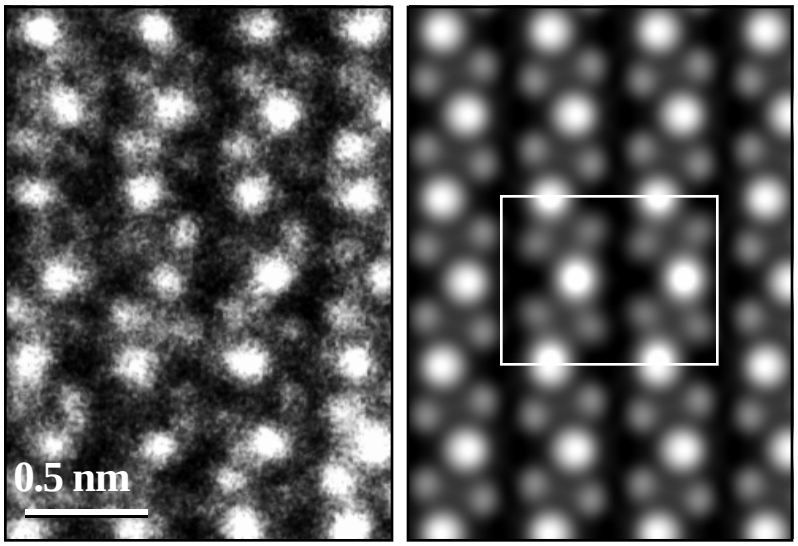
tools for future phase identification and alloy development.



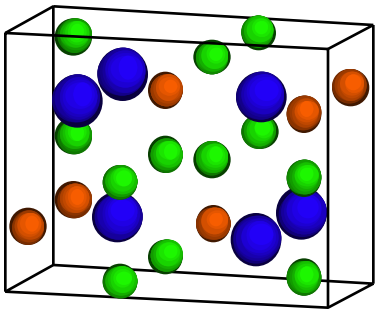
Left: High resolution image of dispersion-strengthening S-phase precipitate embedded in aluminum matrix. The irrational orientation relationship with the matrix apparent from this image was explained from its crystallography. Although the precipitates are only a few nanometers in size, their crystal structure was refined using quantitative analysis as shown below.



Cross correlation map showing peak of 0.9955 for imaging and atomic parameters indicated in the figure and shown in the table below.



Quantitative analysis of high resolution TEM images of S-phase in [100] orientation. Poor signal to noise ratio in unprocessed image (left) is enhanced by crystallographic image processing (right). Inset frame shows best-matching image simulation.



Refined Wyckoff positions

Al	(0.0	0.3622	0.0556)
Cu	(0.0	0.0736	0.25)
Mg	(0.0	0.7650	0.25)

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